

Bis(2-methoxyanilinium) hexabromido-stannate(IV) dihydrate

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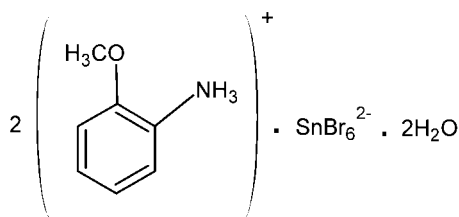
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Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.017$ Å; R factor = 0.061; wR factor = 0.156; data-to-parameter ratio = 16.5.

The asymmetric unit of the title compound, $(\text{C}_7\text{H}_{10}\text{NO})_2\text{[SnBr}_6\text{]}\cdot 2\text{H}_2\text{O}$, contains one cation, one half-dianion and one lattice water molecule. The $[\text{SnBr}_6]^{2-}$ dianion, located on an inversion center, exhibits a highly distorted octahedral coordination environment, with $\text{Sn}-\text{Br}$ bond lengths ranging from 2.2426 (9) to 3.0886 (13) Å. In the crystal, $\text{O}-\text{H}\cdots\text{Br}$, $\text{N}-\text{H}\cdots\text{Br}$, $\text{N}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{Br}$ hydrogen bonds consolidate the packing, which can be described as consisting of alternating anionic (containing dianions and lattice water molecules) and cationic layers parallel to ab plane.

Related literature

For general background to hybrid organic-inorganic compounds, see: Kagan *et al.* (1999); Raptopoulou *et al.* (2002). For related structures, see: Tudela & Khan (1991); Chouaib *et al.* (2013); Benali-Cherif *et al.* (2007); Karoui *et al.* (2013); Guelmami *et al.* (2007); Souissi *et al.* (2011); Smith *et al.* (2006).



Experimental

Crystal data

$(\text{C}_7\text{H}_{10}\text{NO})_2[\text{SnBr}_6]\cdot 2\text{H}_2\text{O}$
 $M_r = 882.50$
 Monoclinic, $P2_1/a$

$a = 10.8728$ (7) Å
 $b = 13.4403$ (10) Å
 $c = 9.0695$ (6) Å

$\beta = 103.680$ (5)°
 $V = 1287.76$ (15) Å³
 $Z = 2$
 Mo $K\alpha$ radiation

$\mu = 10.32$ mm⁻¹
 $T = 293$ K
 $0.10 \times 0.10 \times 0.10$ mm

Data collection

Agilent Xcalibur (Sapphire2) diffractometer
 Absorption correction: multi-scan (*CrysAlis RED*; Agilent, 2012)
 $T_{\min} = 0.356$, $T_{\max} = 0.371$

7762 measured reflections
 2188 independent reflections
 1854 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.052$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.061$
 $wR(F^2) = 0.156$
 $S = 1.07$
 2188 reflections
 133 parameters
 9 restraints

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\max} = 1.51$ e Å⁻³
 $\Delta\rho_{\min} = -1.44$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1}-\text{H1B}\cdots\text{Br2}^{\text{i}}$	0.89	2.82	3.557 (9)	141
$\text{N1}-\text{H1C}\cdots\text{OW}^{\text{ii}}$	0.89	2.63	3.151 (15)	119
$\text{OW}-\text{H1W}\cdots\text{Br2}^{\text{i}}$	0.88 (9)	2.64 (9)	3.457 (9)	154 (11)
$\text{OW}-\text{H2W}\cdots\text{Br1}^{\text{iii}}$	0.88 (9)	2.42 (9)	3.296 (8)	171 (16)
$\text{C7}-\text{H7A}\cdots\text{Br1}^{\text{iii}}$	0.96	2.71	3.459 (15)	135
$\text{N1}-\text{H1A}\cdots\text{Br1}^{\text{ii}}$	0.89	2.75	3.154 (9)	109
$\text{C5}-\text{H5}\cdots\text{Br2}^{\text{iv}}$	0.93	2.52	3.289 (12)	140

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, z$; (iii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+1$; (iv) $-x+1, -y+1, -z$.

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Agilent, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg *et al.*, 1999) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5437).

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supplementary materials

Acta Cryst. (2013). E69, m678–m679 [doi:10.1107/S1600536813031681]

Bis(2-methoxyanilinium) hexabromidostannate(IV) dihydrate

Hassen Chouaib, Sahel Karoui, Slaheddine Kamoun and Francois Michaud

1. Comment

Hybrid organic-inorganic compounds are of great interest owing to their ionic, electrical, magnetic and optical properties (Kagan *et al.*, 1999; Raptopoulou *et al.*, 2002). As a continuation of our structural study of such hydrid compounds containing 2-methoxyanilinium cation (Karoui *et al.*, 2013), we report herein the crystal structure of the title compound (I).

The asymmetric unit of (I) contains one 2-methoxyanilinium cation, one-half dianion and one crystalline water molecule (Fig. 1). The $[\text{SnBr}_6]^{2-}$ dianion located on an inversion center exhibits a highly distorted octahedral coordination environment with Sn—Br bond lengths ranging from 2.2426 (9) Å to 3.0886 (13) Å. The Br—Sn—Br angles for the Br atoms in *cis* positions with respect to each other fall in the range of 83.74 (4) to 96.26 (4)°. The $[\text{SnBr}_6]^{2-}$ dianions interact with water molecules *via* O—H \cdots Br hydrogen bonds (Table 1) thus forming anionic layers parallel to the *ab* plane (Fig. 2). Bond lengths and angles within the cations and dianions are as expected and comparable with those observed in the related compounds (Benali-Cherif *et al.*, 2007; Karoui *et al.*, 2013; Guelmami *et al.*, 2007; Souissi *et al.*, 2011; Smith *et al.*, 2006; Tudela & Khan, 1991; Chouaib *et al.*, 2013). The phenyl ring is practically planar with the greatest deviation from the six-atoms least squares plane being 0.0156 Å. The torsion angle O1—C1—C2—N1 is 2 (2)° indicating that the N1—C2 and C1—O1 groups deviate from the phenyl ring plane. The methoxy group of the organic cation makes an angle of 0(2)° with the plane of the phenyl ring and is in short intramolecular contact with O1 (N \cdots O = 2.824 (14) Å). The benzene ring is regular with C—C—C angles in agreement with the expected sp² hybridization.

In the crystal, intermolecular O—H \cdots Br, N—H \cdots Br, N—H \cdots O and C—H \cdots Br hydrogen bonds (Table 1) consolidate the packing (Fig. 3), which can be described as consisting of alternating anionic (containing dianions and crystalline water molecules) and cationic layers parallel to *ab* plane.

2. Experimental

(C₇H₁₀NO)₂SnBr₆·2H₂O was prepared by refluxing during 5 h a solution of metallic tin (3 g, 25 mmol) in 40 ml an aqueous solution of hydrobromic acid, HBr 47%. To this solution, 9.5 ml (75 mmol) of a solution of 2-methoxyanilin was added at reflux temperature. After a slow solvent evaporation yellow crystals suitable for X-ray analysis were obtained. They were washed with diethyl ether and dried over P₂O₅.

3. Refinement

All H atoms were geometrically positioned and treated as riding on their parent atoms, with C—H = 0.93 Å for the phenyl, 0.96 Å for the methyl and N—H = 0.89 Å with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C-phenyl, N})$ or $1.5 U_{\text{eq}}(\text{C-methyl})$. The water H atoms were located in a difference Fourier map and refined using *DFIX* restraints (O—H 0.88 (7) Å). and a riding model, with $U_{\text{iso}}(\text{H}) = 1.5 U_{\text{eq}}(\text{O})$.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis RED* (Agilent, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg *et al.*, 1999) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

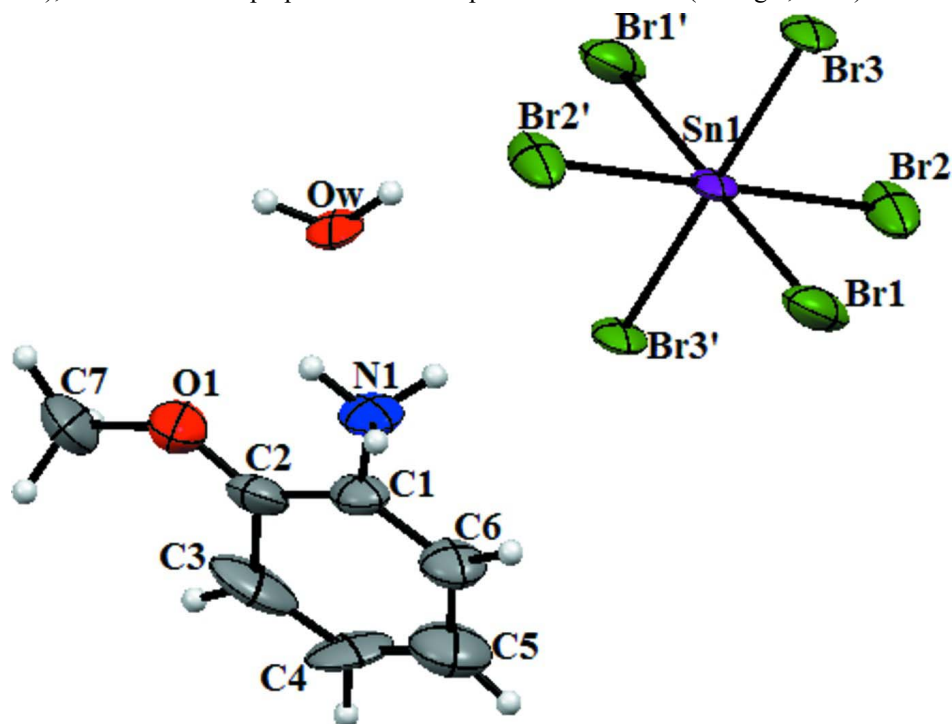


Figure 1

A view of the asymmetric unit of (I) showing the atomic numbering and 50% probability displacement ellipsoids [symmetry code: (i) $-x + 1, -y + 1, -z + 1$].

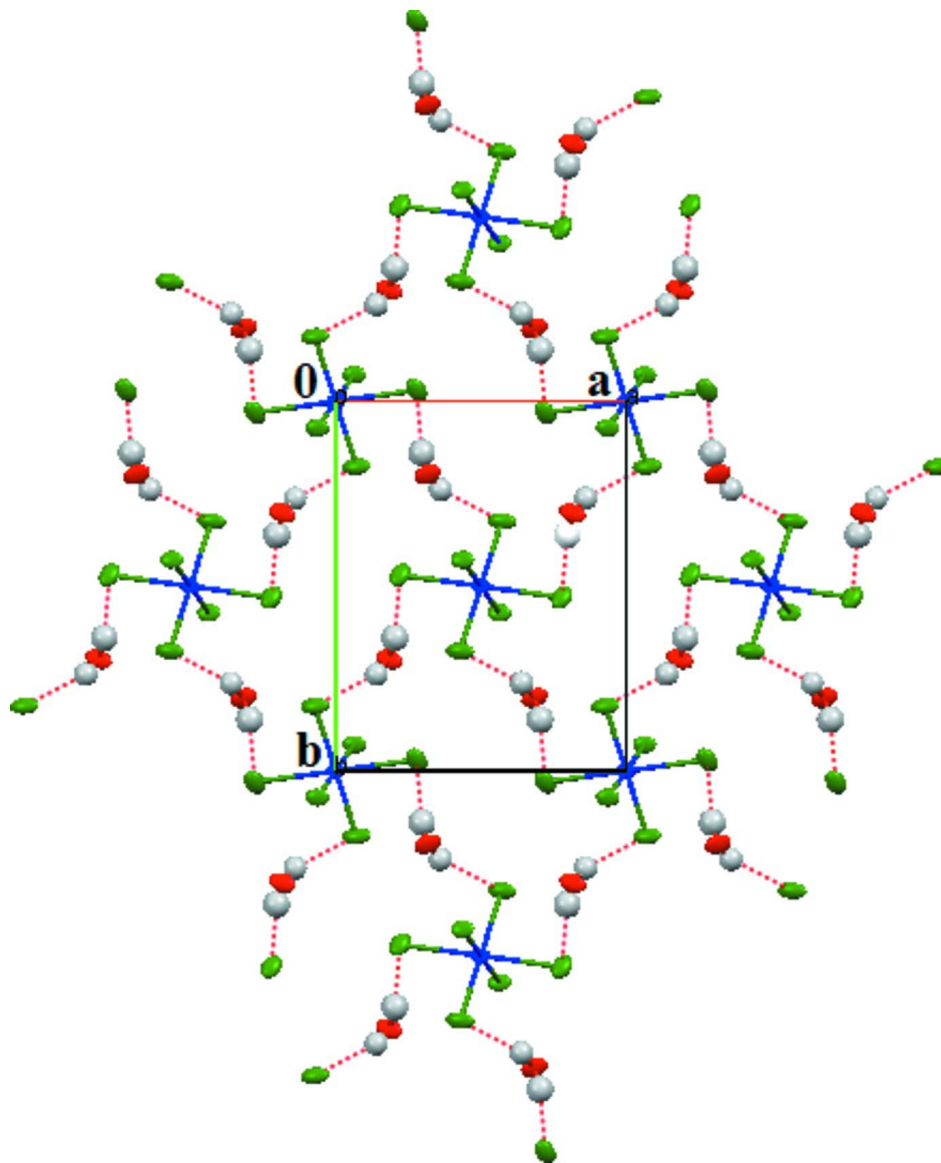
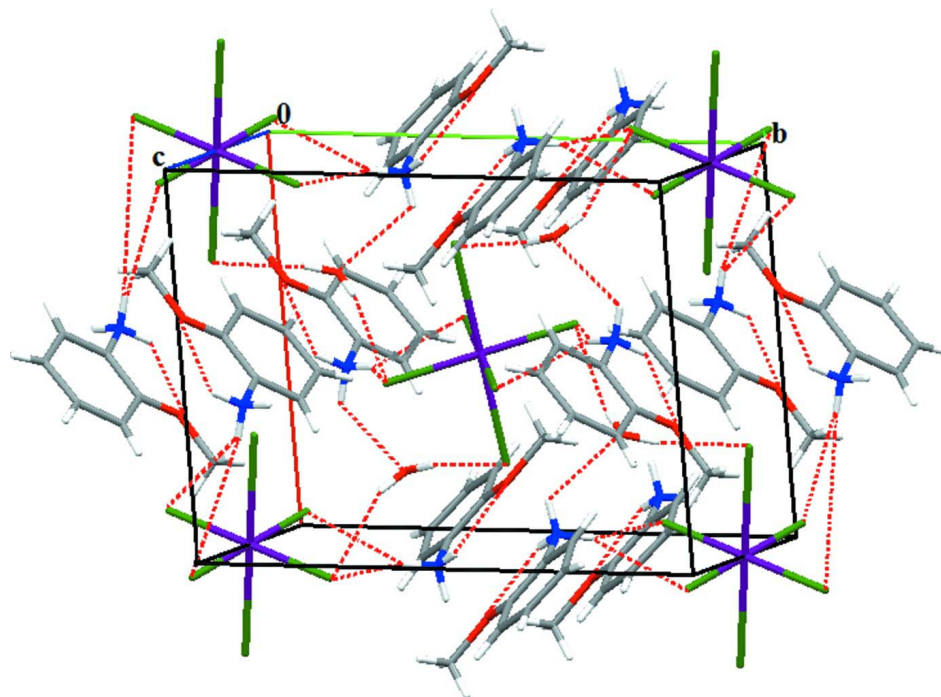


Figure 2

An anionic layer in (I) viewed along the *c* axis. Intermolecular hydrogen bonds are shown as red dashed lines.

**Figure 3**

A portion of the crystal packing showing the hydrogen bonds as red dashed lines.

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Crystal data

$(C_7H_{10}NO)_2[SnBr_6] \cdot 2H_2O$

$M_r = 882.50$

Monoclinic, $P2_1/a$

Hall symbol: $-P\ 2yab$

$a = 10.8728\ (7)\ \text{\AA}$

$b = 13.4403\ (10)\ \text{\AA}$

$c = 9.0695\ (6)\ \text{\AA}$

$\beta = 103.680\ (5)^\circ$

$V = 1287.76\ (15)\ \text{\AA}^3$

$Z = 2$

$F(000) = 828$

$D_x = 2.276\ \text{Mg m}^{-3}$

$D_m = 2.276\ \text{Mg m}^{-3}$

D_m measured by not measured

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 5970 reflections

$\theta = 3.6\text{--}24.7^\circ$

$\mu = 10.32\ \text{mm}^{-1}$

$T = 293\ \text{K}$

Prism, yellow

$0.10 \times 0.10 \times 0.10\ \text{mm}$

Data collection

Agilent Xcalibur (Sapphire2)

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

Absorption correction: multi-scan

(*CrysAlis RED*; Agilent, 2012)

$T_{\min} = 0.356$, $T_{\max} = 0.371$

7762 measured reflections

2188 independent reflections

1854 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.052$

$\theta_{\max} = 24.7^\circ$, $\theta_{\min} = 3.6^\circ$

$h = -12 \rightarrow 12$

$k = -11 \rightarrow 15$

$l = -10 \rightarrow 10$

2 standard reflections every 120 min

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.061$
 $wR(F^2) = 0.156$
 $S = 1.07$

2188 reflections

133 parameters

9 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H atoms treated by a mixture of independent
and constrained refinement

 $w = 1/[\sigma^2(F_o^2) + (0.0686P)^2 + 18.8968P]$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 1.51 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -1.44 \text{ e } \text{\AA}^{-3}$

Extinction correction: *SHELXL97* (Sheldrick,
2008), $F_c^* = kF_c[1 + 0.001 \times F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0039 (8)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn1	0.5000	0.5000	0.5000	0.0316 (4)
Br2	0.42826 (15)	0.67591 (9)	0.41106 (12)	0.0609 (5)
Br3	0.56362 (12)	0.57192 (8)	0.72849 (10)	0.0444 (4)
Br1	0.22150 (13)	0.46965 (11)	0.51438 (14)	0.0582 (5)
OW	0.3159 (10)	0.1977 (7)	0.3700 (8)	0.056 (2)
N1	0.5673 (10)	0.1749 (8)	0.2638 (9)	0.047 (2)
H1A	0.5324	0.1285	0.3109	0.071*
H1B	0.5596	0.2341	0.3048	0.071*
H1C	0.6489	0.1611	0.2738	0.071*
O1	0.3632 (11)	0.0449 (7)	0.1485 (10)	0.068 (3)
C1	0.5131 (11)	0.1763 (8)	0.1279 (11)	0.043 (3)
C2	0.4114 (12)	0.1068 (9)	0.0787 (10)	0.050 (3)
C6	0.5699 (11)	0.2478 (9)	0.0605 (10)	0.052 (3)
H6	0.6399	0.2847	0.1101	0.063*
C4	0.4156 (15)	0.1880 (12)	−0.1337 (13)	0.072 (4)
H4	0.3809	0.1929	−0.2375	0.086*
C7	0.2509 (19)	−0.0282 (12)	0.0978 (18)	0.081 (5)
H7A	0.2398	−0.0658	0.1838	0.122*
H7B	0.2682	−0.0728	0.0225	0.122*
H7C	0.1751	0.0086	0.0557	0.122*
C3	0.3580 (13)	0.1144 (11)	−0.0702 (11)	0.077 (5)
H3	0.2914	0.0753	−0.1227	0.092*
C5	0.5122 (16)	0.2580 (13)	−0.0858 (11)	0.081 (5)
H5	0.5338	0.3061	−0.1489	0.097*

H1W	0.360 (10)	0.238 (7)	0.439 (10)	0.08 (5)*
H2W	0.297 (16)	0.139 (6)	0.402 (14)	0.10 (6)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0520 (7)	0.0323 (6)	0.0091 (5)	0.0004 (4)	0.0045 (4)	−0.0037 (3)
Br2	0.1150 (12)	0.0381 (7)	0.0191 (6)	0.0070 (6)	−0.0052 (6)	0.0030 (4)
Br3	0.0776 (9)	0.0429 (7)	0.0101 (5)	−0.0015 (5)	0.0054 (5)	−0.0050 (4)
Br1	0.0642 (8)	0.0749 (9)	0.0411 (7)	−0.0200 (7)	0.0237 (6)	−0.0303 (6)
OW	0.099 (7)	0.055 (5)	0.015 (3)	−0.019 (5)	0.015 (4)	0.005 (3)
N1	0.065 (6)	0.057 (6)	0.018 (4)	0.006 (5)	0.005 (4)	0.007 (4)
O1	0.106 (8)	0.061 (6)	0.038 (5)	−0.027 (5)	0.021 (5)	−0.010 (4)
C1	0.060 (7)	0.048 (6)	0.020 (5)	0.007 (5)	0.010 (5)	0.004 (4)
C2	0.066 (8)	0.059 (8)	0.031 (6)	−0.001 (6)	0.021 (5)	−0.016 (5)
C6	0.066 (8)	0.063 (8)	0.023 (5)	0.001 (6)	0.000 (5)	0.000 (5)
C4	0.088 (10)	0.113 (13)	0.016 (5)	0.000 (9)	0.015 (6)	0.020 (7)
C7	0.131 (15)	0.061 (9)	0.057 (9)	−0.034 (9)	0.035 (9)	−0.032 (7)
C3	0.068 (9)	0.113 (13)	0.041 (7)	0.001 (9)	−0.004 (6)	−0.048 (8)
C5	0.104 (12)	0.100 (12)	0.035 (7)	−0.003 (10)	0.010 (7)	−0.012 (8)

Geometric parameters (\AA , $^\circ$)

Sn1—Br3	2.2426 (9)	O1—C7	1.550 (18)
Sn1—Br3 ⁱ	2.2426 (9)	C1—C6	1.363 (9)
Sn1—Br2	2.5595 (11)	C1—C2	1.437 (16)
Sn1—Br2 ⁱ	2.5595 (11)	C2—C3	1.341 (9)
Sn1—Br2 ⁱ	2.5595 (11)	C6—C5	1.333 (9)
Sn1—Br1	3.0886 (13)	C6—H6	0.9300
Sn1—Br1 ⁱ	3.0886 (13)	C4—C3	1.368 (9)
OW—H1W	0.88 (9)	C4—C5	1.40 (2)
OW—H2W	0.88 (9)	C4—H4	0.9300
N1—C1	1.234 (13)	C7—H7A	0.9600
N1—H1A	0.8900	C7—H7B	0.9600
N1—H1B	0.8900	C7—H7C	0.9600
N1—H1C	0.8900	C3—H3	0.9300
O1—C2	1.235 (14)	C5—H5	0.9300
Br3—Sn1—Br3 ⁱ	180.0	H1B—N1—H1C	109.5
Br3—Sn1—Br2	84.12 (4)	C2—O1—C7	132.4 (11)
Br3 ⁱ —Sn1—Br2	95.88 (4)	N1—C1—C6	107.4 (10)
Br3—Sn1—Br2 ⁱ	95.88 (4)	N1—C1—C2	116.8 (9)
Br3 ⁱ —Sn1—Br2 ⁱ	84.12 (4)	C6—C1—C2	135.8 (9)
Br2—Sn1—Br2 ⁱ	180.0	O1—C2—C3	115.7 (12)
Br3—Sn1—Br2 ⁱ	95.88 (4)	O1—C2—C1	131.9 (9)
Br3 ⁱ —Sn1—Br2 ⁱ	84.12 (4)	C3—C2—C1	112.4 (10)
Br2—Sn1—Br2 ⁱ	180.0	C5—C6—C1	111.2 (11)
Br2 ⁱ —Sn1—Br2 ⁱ	0.00 (5)	C5—C6—H6	124.4
Br3—Sn1—Br1	96.26 (4)	C1—C6—H6	124.4
Br3 ⁱ —Sn1—Br1	83.74 (4)	C3—C4—C5	137.6 (11)

Br2—Sn1—Br1	84.64 (5)	C3—C4—H4	111.2
Br2 ⁱ —Sn1—Br1	95.36 (5)	C5—C4—H4	111.2
Br2 ⁱ —Sn1—Br1	95.36 (5)	O1—C7—H7A	109.5
Br3—Sn1—Br1 ⁱ	83.74 (4)	O1—C7—H7B	109.5
Br3 ⁱ —Sn1—Br1 ⁱ	96.26 (4)	H7A—C7—H7B	109.5
Br2—Sn1—Br1 ⁱ	95.36 (5)	O1—C7—H7C	109.5
Br2 ⁱ —Sn1—Br1 ⁱ	84.64 (5)	H7A—C7—H7C	109.5
Br2 ⁱ —Sn1—Br1 ⁱ	84.64 (5)	H7B—C7—H7C	109.5
Br1—Sn1—Br1 ⁱ	180.00 (5)	C2—C3—C4	110.3 (10)
H1W—OW—H2W	116.9 (4)	C2—C3—H3	124.8
C1—N1—H1A	109.5	C4—C3—H3	124.8
C1—N1—H1B	109.5	C6—C5—C4	112.5 (12)
H1A—N1—H1B	109.5	C6—C5—H5	123.8
C1—N1—H1C	109.5	C4—C5—H5	123.8
H1A—N1—H1C	109.5		
C7—O1—C2—C3	0 (2)	C2—C1—C6—C5	4 (2)
C7—O1—C2—C1	177.8 (14)	O1—C2—C3—C4	177.3 (13)
N1—C1—C2—O1	2 (2)	C1—C2—C3—C4	−0.6 (17)
C6—C1—C2—O1	−178.2 (15)	C5—C4—C3—C2	−2 (3)
N1—C1—C2—C3	179.6 (12)	C1—C6—C5—C4	−4.5 (19)
C6—C1—C2—C3	−1 (2)	C3—C4—C5—C6	5 (3)
N1—C1—C6—C5	−176.6 (13)		

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1B \cdots Br2 ⁱ	0.89	2.82	3.557 (9)	141
N1—H1C \cdots OW ⁱⁱ	0.89	2.63	3.151 (15)	119
OW—H1W \cdots Br2 ⁱ	0.88 (9)	2.64 (9)	3.457 (9)	154 (11)
OW—H2W \cdots Br1 ⁱⁱⁱ	0.88 (9)	2.42 (9)	3.296 (8)	171 (16)
C7—H7A \cdots Br1 ⁱⁱⁱ	0.96	2.71	3.459 (15)	135
N1—H1A \cdots Br1 ⁱⁱ	0.89	2.75	3.154 (9)	109
C5—H5 \cdots Br2 ^{iv}	0.93	2.52	3.289 (12)	140

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x+1/2, -y+1/2, z$; (iii) $-x+1/2, y-1/2, -z+1$; (iv) $-x+1, -y+1, -z$.